

Nagaoka ferromagnetism in large-spin systems

-Fermion and Boson systems-

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Abstract

We study magnetic properties of itinerant quantum magnetic particles described by a generalized Hubbard model with large spin ($S > 1/2$) which may be realized in optical lattices of laser-cooled atom systems. In fermion systems (half-integer spins), an extended form of Nagaoka ferromagnetism may be realized. However, as novel aspects of the large spin cases, we found that the condition on the lattice connectivity is more stringent than in the case of $S = 1/2$ particles, and that the system shows a peculiar degenerate structure of the ground state in which the ferromagnetic state is included. In contrast, it turns out that the ground state of itinerant bosonic systems (integer spins) has a degenerate structure similar to that of fermion system with $S > 1/2$ regardless of the shape, connectivity or filling of the lattice, and that the state with the maximum total spin is always one of the ground states.

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I. INTRODUCTION

The origin of magnetism is attributed to the quantum mechanical interaction of particles which carry spin. In so-called localized spin systems, the Pauli principle plays an essential role and the magnetic interaction is expressed as the Heisenberg interaction¹, the exchange integral between atoms being the dominant term. Not only the two-spin interaction but also multi-spin interactions may contribute to give rise to exotic magnetic states. In particular, various effects of the multi-spin interaction have been reported in $^3\text{He}^2$. For itinerant electron systems, the origin of the magnetic order, and of ferromagnetic order in particular, has been studied extensively. Itinerant electron systems are often described by tight binding models such as the Hubbard model⁴. Nagaoka pointed out that the ground state of the Hubbard model may be a ferromagnetic state (Nagaoka ferromagnetic state) if the number of electrons is reduced by one from half-filling^{5,6}, where half-filling means that the number of particles is the same as the number of the lattice sites. The Nagaoka ferromagnetic state is established if the so-called “connectivity condition” on the lattice is satisfied^{5,8}. In the Nagaoka ferromagnetic state, the energy of the system is minimized when the total spin of the system takes the maximum value. On the other hand, the ground state of the half filled system is a singlet state, that is its total spin is zero. Elsewhere, we have studied how the magnetic state changes between these two states when an electron is removed from the system and demonstrated an adiabatic change between these states⁹.

Magnetism has primarily been studied in electron systems in which the spin $S = 1/2$. However, recently developments in the field of laser-cooled atomic systems have opened new possibilities to realize artificial tight-binding quantum system such as the Hubbard model^{10,11}. In contrast to electron systems, in optical lattices the spin of trapped atoms is not necessarily $S = 1/2$ but can take larger half-integer or integer values. In the latter case, the system contains bosons, not fermions, and it is therefore of interest to study itinerant magnetism of systems with $S > 1/2$. The present paper presents the results of such systems.

II. MODEL

We consider a tight binding model of the form

$$\mathcal{H} = -t \sum_{\langle ij \rangle, M} \left(c_{i,M}^\dagger c_{j,M} + c_{j,M}^\dagger c_{i,M} \right) + \sum_{i=1}^N U(n_{i,M}), \quad (1)$$

where $c_{i,M}^\dagger$ and $c_{i,M}$ are the annihilation and creation operators of a particle (fermion or boson depending on its spin) of the magnetization M at a site i , respectively, $n_{i,M}$ is the number operator

$$n_{i,M} = c_{i,M}^\dagger c_{i,M}, \quad (2)$$

for the particle of spin S , $M = -S, -S+1, \dots, S$, and $U(n_{i,M})$ represents the on-site repulsive interaction. For the system with $S = 1/2$, we take for $U(n_{i,M})$ the standard form

$$U(n_{i,M}) = U_0 n_{i,-1/2} n_{i,1/2}, \quad (3)$$

and for larger $S > 1/2$ we extend it as

$$U(n_{i,M}) = \frac{1}{2} U_0 N_i (N_i - 1), \quad (4)$$

where $N_i = \sum_M n_{i,M}$ and U_0 is assumed to be positive. Obviously, the interaction $U(n_{i,M})$ increases the energy whenever a site is occupied by more than one particle.

In order to study magnetic properties of the system, we introduce spin operators for the magnetization $\mathbf{S} = (S_i^x, S_i^y, S_i^z)$ of the particles, where

$$S_i^z = \sum_{M=-S}^S M n_{i,M}. \quad (5)$$

Hereafter, we use the operators $S_i^+ = S_i^x + iS_i^y$ and $S_i^- = S_i^x - iS_i^y$ which are expressed in terms of $c_{i,M}^\dagger$ and $c_{i,M}$:

$$S_i^+ = \sum_M \sqrt{(S-M)(S+M+1)} c_{i,M+1}^\dagger c_{i,M} \quad (6)$$

and

$$S_i^- = \sum_M \sqrt{(S+M)(S-M+1)} c_{i,M-1}^\dagger c_{i,M}, \quad (7)$$

where S is the total spin of each particle, and M is the z -component of the magnetization. To discuss the magnetic properties of the states, we adopt the usual notation $|S, M\rangle$ where

S is the total spin S and M is the magnetization. The action of the operators Eqs. (6) and (7) on the state $|S, M\rangle$ is given by the relations

$$S_i^+ |S, M\rangle = \sqrt{(S - M)(S + M + 1)} |S, M + 1\rangle \quad (8)$$

and

$$S_i^- |S, M\rangle = \sqrt{(S + M)(S - M + 1)} |S, M - 1\rangle. \quad (9)$$

In order to explicitly compute matrix elements of the operators, it is convenient to introduce orthonormal basis states. In the case of fermion systems, we adopt the form

$$|\Psi\rangle = c_{i,M}^\dagger \cdots c_{j,M'}^\dagger |0\rangle, \quad (10)$$

where $i \geq j$, and $M > M'$ if $i = j$. With this definition, the operations Eqs. (6) and (7) do not change the order of creation operators in Eq. (10). In the case of bosons, more than two particles with the same M can occupy the same site and the normalized basis states take the form

$$|\Psi\rangle = \frac{(c_{i,M}^\dagger)^{n_{i,M}} \cdots (c_{j,M'}^\dagger)^{n_{j,M'}} |0\rangle}{\sqrt{n_{i,M}!} \cdots \sqrt{n_{j,M'}!}} \equiv |n_{i,M}\rangle \cdots |n_{j,M'}\rangle. \quad (11)$$

For boson systems, the order of i and j and M and M' is not relevant.

The total spin of the whole system is given by

$$\mathbf{S}^2 = (S^x)^2 + (S^y)^2 + (S^z)^2 = \frac{S^+ S^- + S^- S^+}{2} + (S^z)^2, \quad (12)$$

where $S^x = \sum_i S_i^x$, $S^y = \sum_i S_i^y$, and $S^z = \sum_i S_i^z$, and $S^\pm = \sum_i S_i^x \pm i S_i^y$. We denote the value of the total spin of the system by S_{tot} , i.e., $S_{\text{tot}}(S_{\text{tot}} + 1) = \langle \mathbf{S}^2 \rangle$.

III. CONSERVATION OF NUMBER OF PARTICLES OF DIFFERENT SPINS AND GROUND-STATE DEGENERACY

It should be noted that the Hubbard Hamiltonian conserves number of particles

$$n_M = \sum_{i=1}^N n_{i,M} \quad (13)$$

for each M . To describe the set of n_M of states, it is convenient to introduce the notation

$$\{n_M\} = (n_S, n_{S-1}, \cdots, n_{-S}), \quad (14)$$

where $\sum_{M=-S}^{+S} n_M = N$. It is important to note that except for $S = 1/2$, the operator $S_i^+ S_j^- + S_i^- S_j^+$ changes the set $\{n_M\}$. For example, if $S = 1$ application of $S_i^+ S_j^- + S_i^- S_j^+$ to states in the set $(n_1 = 0, n_0 = 2, n_{-1} = 0)$, created states in the set $(n_1 = 1, n_0 = 0, n_{-1} = 1)$. Thus, except for $S = 1/2$, the matrix element $\langle \{n'_M\} | S_i^+ S_j^- + S_i^- S_j^+ | \{n_M\} \rangle$ can be nonzero even if $\{n_M\} \neq \{n'_M\}$.

Thus, even though the Hamiltonian \mathcal{H} has the $SU(2)$ symmetry, conserves the total spin, and therefore commutes with S^\pm , the operation of $S_i^+ S_j^- + S_i^- S_j^+$ on each state with given $\{n_M\}$ must be treated carefully.

Let us denote by $|G, M\rangle$ the ground state in the space with the magnetization M . Because the Hamiltonian \mathcal{H} and S^\pm commute with each other, $S^-|G, M\rangle$ is also a ground state because

$$\mathcal{H}S^-|G, M\rangle = S^-\mathcal{H}|G, M\rangle = E_G S^-|G, M\rangle. \quad (15)$$

However, the set of numbers $\{n_M\}$ is not necessarily conserved, that is

$$\begin{aligned} S^-\mathcal{H}|G, M, \{n_M\}\rangle &= E_G S^-|G, M, \{n_M\}\rangle \\ &= E_G \sum_{\{n'_M\}} a_{\{n'_M\}} |G, M-1, \{n'_M\}\rangle, \end{aligned} \quad (16)$$

where $|G, M, \{n_M\}\rangle$ denotes one of basis states with fixed $\{n_M\}$ that contribute to the expansion of $|G, M\rangle$ in terms of basis states. The energy of this state is given by

$$\begin{aligned} E_G &= \frac{\langle G, M, \{n_M\} | S^+ \mathcal{H} S^- | G, M, \{n_M\} \rangle}{\langle G, M, \{n_M\} | S^+ S^- | G, M, \{n_M\} \rangle} \\ &= \frac{\sum_{\{n'_M\}} |a_{\{n'_M\}}|^2 \langle G, M-1, \{n'_M\} | \mathcal{H} | G, M-1, \{n'_M\} \rangle}{\sum_{\{n'_M\}} |a_{\{n'_M\}}|^2 \langle G, M-1, \{n'_M\} | G, M-1, \{n'_M\} \rangle}. \end{aligned} \quad (17)$$

Because

$$\frac{\langle G, M-1, \{n'_M\} | \mathcal{H} | G, M-1, \{n'_M\} \rangle}{\langle G, M-1, \{n'_M\} | G, M-1, \{n'_M\} \rangle} \geq E_G, \quad (18)$$

in order to satisfy the relation (17), the state in each set of numbers $\{n'_M\}$ must be the ground state, i.e.

$$\frac{\langle G, M-1, \{n'_M\} | \mathcal{H} | G, M-1, \{n'_M\} \rangle}{\langle G, M-1, \{n'_M\} | G, M-1, \{n'_M\} \rangle} = E_G, \quad (19)$$

and thus

$$\mathcal{H}|G, M-1, \{n'_M\}\rangle = E_G |G, M-1, \{n'_M\}\rangle. \quad (20)$$

This shows that the same ground state energy is found for all sets $\{n'_M\}$ except if $a_{\{n'_M\}} = 0$.

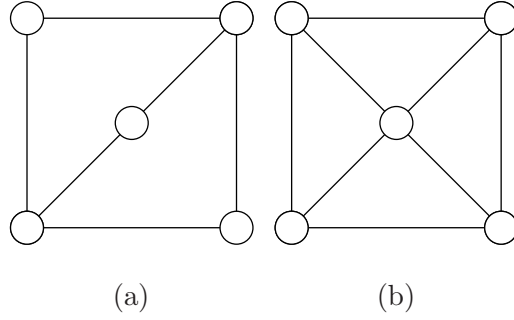


FIG. 1: Lattices: (a) five sites and six bonds; (b) lattice (a) with two additional bonds.

IV. GROUND STATE OF A FERMION SYSTEM WITH $S = \frac{3}{2}$

A. Subspaces due to conservation of particle number of each M

Let us now study the dependence of the ground state energy on U_0 . We consider a system with four particles with $S = 3/2$ on the 5-site lattice depicted in Fig. 1(a). Figure 2(a) shows the ground state energies for the sets $\{n_M\} = (n_{3/2}, n_{1/2}, n_{-1/2}, n_{-3/2}) = (4, 0, 0, 0), (3, 1, 0, 0), (2, 2, 0, 0), (2, 1, 1, 0), (1, 1, 1, 1)$, corresponding to systems in which the number of different states is 5, 50, 100, 250 and 625, respectively. The Hamiltonian does not depend on the values of M , and thus the energy level structure is same for the cases with the same set of numbers, e.g. for $(3, 1, 0, 0), (3, 0, 1, 0), \dots, (0, 0, 1, 3)$. For small value of U_0 , the ground state energies are all different. As U_0 increases, the ground state energies of $(3, 1, 0, 0)$, $(2, 2, 0, 0)$ and $(2, 1, 1, 0)$ become degenerate with that of $(4, 0, 0, 0)$. This fact indicates that the lowest energy state in these sets has the total spin S_{\max} . However, we find that the lowest energy state in the set $(1, 1, 1, 1)$ is always lower than that of $(4, 0, 0, 0)$. This means that even at large U_0 the ground state has total spin $S < S_{\max}$. Therefore, the Nagaoka-ferromagnetic state, i.e., the state of the maximum total spin, is not realized as the ground state in the present case even at large values of U_0 .

In general, when there are multiple conserved quantities in a system that do not commute with each other, each energy state of the system is usually degenerate as shown in Eq. (20)¹². In the present model, the total magnetization and the set $\{n_M\}$ are conserved. However, the ground state in Fig. 2(a) is not degenerate, which gives an exception to the above general property.

Figure 3 shows the U_0 dependence of the total spin of the lowest-energy state for the

sets $\{n_M\}$ on the lattice of Fig. 2(a). The total spin of states in the subspace (4,0,0,0) is $S_{\max} = (3/2) \times 4 = 6$. For small values of U , the total spin of states in the subspace (3,1,0,0) is less than S_{\max} , but it becomes S_{\max} when the ground state energy becomes degenerate to that of the (4,0,0,0) subspace. The ground state energies of (2,2,0,0) and (2,1,1,0) become degenerate to that of (4,0,0,0) at certain values of U_0 . However, the total spin of the lowest-energy state of these sets does not reach S_{\max} . This fact agrees with the earlier argument that if $S^-|G, M\rangle$ consists of more than one set of $\{n_M\}$'s, neither of these sets yields an eigenstate of the total spin although each of them have the same ground state energy. Therefore, the expectation value of the total spin is not necessarily an integer.

B. Connectivity condition for the system with $S = \frac{3}{2}$

Note that the lattice shown in Fig. 1(a) satisfies the so-called connectivity condition for the case of $S = 1/2$ and the Nagaoka-ferromagnetic state is realized at large U_0 . However, for $S = 3/2$, this state is not realized. The reason is that the connectivity condition for four $S = 3/2$ particles with different magnetization, i.e., $M = -3/2, -1/2, 1/2, 3/2$ is not satisfied in the lattice of Fig. 1(a). Indeed, the configuration depicted in Fig. 4(a) can not be changed into that of Fig. 4(b).

In order to re-establish the connectivity condition we may add bonds and construct the lattice depicted in Fig. 1(b). This lattice has loops with an odd number of bonds and therefore we need to use a negative value of t . Then, we find that the Nagaoka-ferromagnetic state is realized, as is clear from Fig. 2(b). Summarizing, we have shown that $S = 3/2$ itinerant particle systems may exhibit Nagaoka-ferromagnetism although it is more difficult to satisfy the connectivity condition.

C. Structure of the ground state

We found that the ground state in each subspace for a set $\{n_M\}$ is unique but in each subspace we have one state with the same ground-state energy. In Table I, we list all the sets $\{n_M\}$. The structure indicates that there is a state with $S_{\text{tot}} = 6, 4, 2$ and 0. In the case of $S = 1/2$, there is a one-to-one correspondence between the magnetization M and $\{n_+, n_-\}$, as is clear from Table I. Thus, when we create states by applying S^- from the all-up state,

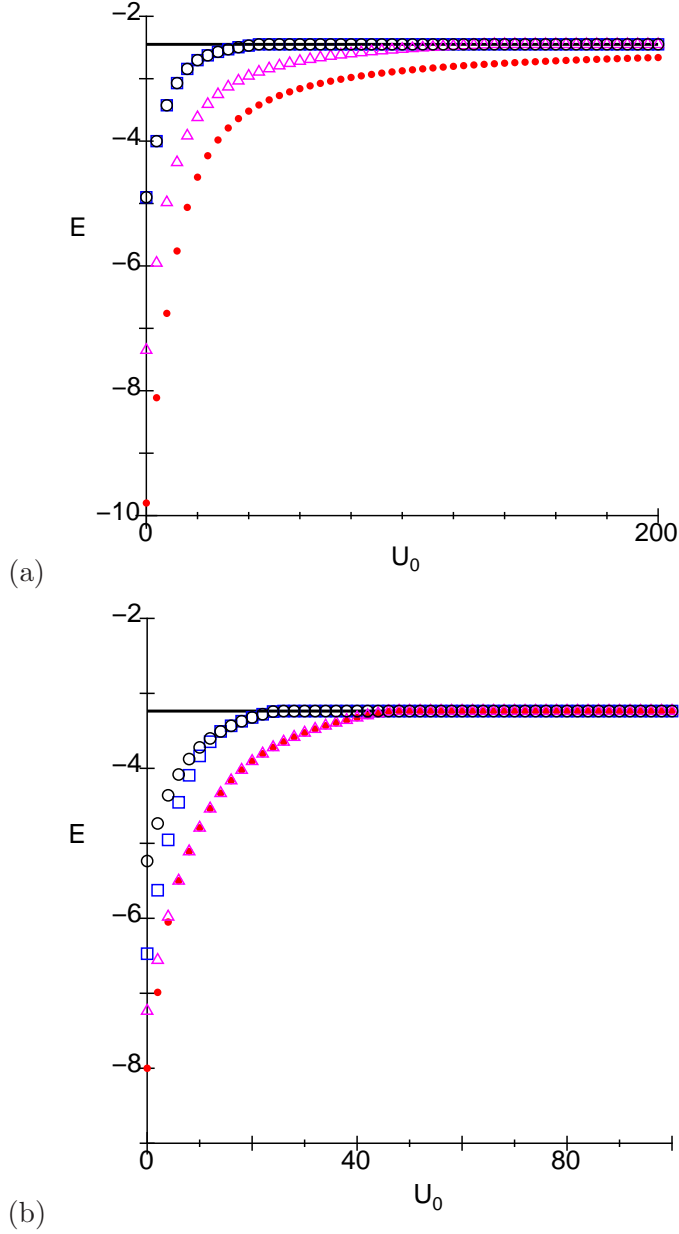


FIG. 2: Energies of the ground state for several sets of $(n_{3/2}, n_{1/2}, n_{-1/2}, n_{-3/2})$. (a) A system with four particles on the lattice shown in Fig. 1(a). The solid line denotes the ground state energy for $(4, 0, 0, 0)$, circles: $(3, 1, 0, 0)$, squares: $(2, 2, 0, 0)$, triangles: $(2, 1, 1, 0)$, and bullets: $(1, 1, 1, 1)$. (b) Same as (a) but for the lattice shown in Fig. 1(b).

we have only the state with $S_{\text{tot}} = 2$ for the four spin system. In contrast, in the case of $S = 3/2$, we create different sets by applying S^- . As we mentioned in the previous section, the created states are degenerate as ground states. Therefore, the structure displayed in

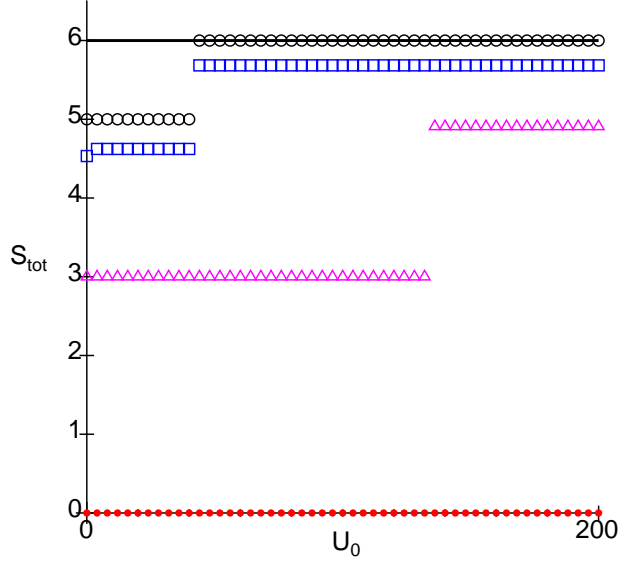


FIG. 3: The total spin S_{tot} of the lowest-energy state for the cases shown in Fig.2(a). The legend is the same as in Fig.2.

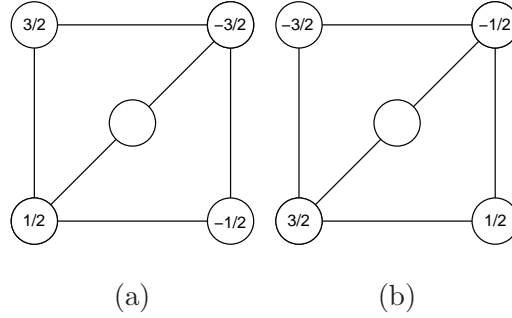


FIG. 4: Nearest-neighbor hopping cannot change configuration (a) into (b) without creating double occupancy.

Table I is intrinsic for systems with $S = 3/2, 5/2, \dots$

V. GROUND STATE OF A BOSON SYSTEM WITH $S = 1$

Next, we study a system of $S = 1$ particles, namely a boson system. Figure 5 shows the ground state energies for the sets $\{n_M\} = (n_1, n_0, n_{-1}) = (4, 0, 0), (0, 4, 0), (3, 1, 0), (3, 0, 1), (2, 2, 0), (2, 1, 1), (1, 2, 1)$, corresponding to systems in which the number of different states is 70, 70, 175, 175, 225, 375, and 375, respectively. Surprisingly, we find that the energies are

TABLE I: Sets of particles of different $M(\geq 0)$ $\{n_M\}$ for the cases of $S = 3/2$ and $1/2$. For $S = 3/2$, we list the sets only for positive M .

$S = 3/2$							
M	6	5	4	3	2	1	0
$\{n_M\}$	(4,0,0,0)	(3,1,0,0)	(3,0,1,0)	(3,0,0,1)	(0,4,0,0)	(0,3,1,0)	(1,0,3,0)
			(2,2,0,0)	(1,3,0,0)	(2,1,0,1)	(2,0,1,1)	(0,3,0,1)
				(2,1,1,0)	(1,2,1,0)	(1,2,0,1)	(2,0,0,2)
					(2,0,2,0)	(1,1,2,0)	(0,2,2,0)
							(1,1,1,1)
$S = 1/2$							
M	2	1	0	-1	2		
$\{n_M\}$	(4,0)	(3,1)	(2,2)	(1,3)	(0,4)		

TABLE II: Sets of particles of different $M(\geq 0)$ $\{n_M\}$ for the case of $S = 1$.

$S = 1$					
M	4	3	2	1	0
$\{n_M\}$	(4,0,0)	(3,1,0)	(3,0,1)	(2,1,1)	(0,4,0)
			(2,2,0)	(1,3,0)	(2,0,2)
					(1,2,1)

the same for all the cases regardless of U_0 . The total spin of the different ground states are also plotted in Fig. 5. Thus, the magnetic properties of the boson system are very different from that of the fermion system. The total spins are less than the maximum value ($S_{\text{tot}}=4$) except for (4,0,0) and (3,1,0) which reflects the fact that the eigenstate of maximum total spin contains more than two sets of $\{n_M\}$, as in the case of the $S = 3/2$ system.

We find a ground state in each set as in the case of $S = 3/2$. We list the sets in Table II. Here we find again a degenerate ground states with $S_{\text{tot}} = 4, 2$ and 0 , which is an intrinsic property of systems with $S = 1, 2, \dots$

Moreover, we find that even in the half-filled case, in the boson system the total spin takes the maximum value. For instance, for a system of four atoms on a simple square

lattice (corresponding to the half-filled case), the ground state is the same for all sets $\{n_M\}$ (results not shown).

This property of boson systems can be understood as follows. Consider the subspace for a fixed set $\{n_M\}$. All the off-diagonal matrix elements of the Hamiltonian \mathcal{H} are $-t$ or 0. By subtracting an appropriate multiple of the unit matrix, also the diagonal elements can be made negative or zero. Thus, all the elements of the shifted matrix \tilde{H} are either negative or zero. In our model, all the sites are connected by bonds and therefore there exist a number $n > 0$ such that all the elements of \tilde{H}^{2n} are positive. Then, the Perron-Frobenius theorem tells us that there exist a unique eigenstate of \tilde{H}^{2n} with an eigenvalue that is larger than the absolute value of all other eigenvalues. This unique eigenstate is therefore the ground state of H , is totally symmetric with positive coefficients, and contains the state of the maximum total spin. However, as we mentioned above, this ground state has an intrinsic degeneracy with respect to subspaces that have different $\{n_M\}$ because we always start from the state with all spins maximum and let S^- create different sets of $\{n'_M\}$. The states that are generated in this manner have all positive coefficients and are therefore ground states too. Clearly, this property does not depend on the connectivity of the lattice or the value of U_0 .

In contrast, for fermion systems, it is in general impossible to transform H such that all elements have the same sign but in those cases for which such a transformation exist, which is precisely the condition of Nagaoka ferromagnetism, we can apply the same arguments as in the boson case to prove that the ground state of H is totally symmetric with positive coefficients and contains the state of the maximum total spin.

VI. SUMMARY AND DISCUSSION

We have studied the magnetic properties of the ground state of itinerant systems with $S > 1$. We found that fermion systems ($S = 3/2$) support an extended form of Nagaoka ferromagnetism but that the connectivity condition is more difficult to satisfy because of the presence of particles with different magnetization. When the maximum S_{tot} state is the ground state, the system has a degenerate ground state in each set $\{n_M\}$ listed in Table I. Thus the ground state manifold consists of not only the state of the maximum S_{tot} but also of states with smaller values of S_{tot} . This degenerate structure is intrinsic for the systems

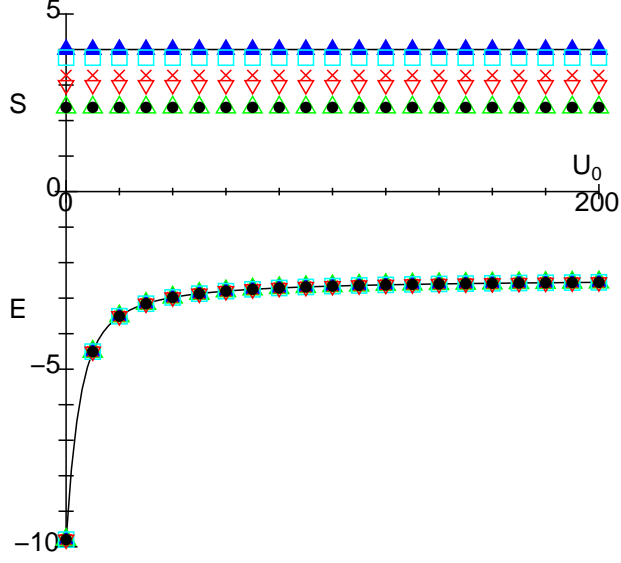


FIG. 5: Ground state energies E and the corresponding total spin S_{tot} as a function of U_0 for four $S = 1$ bosons and various (n_1, n_0, n_{-1}) on the lattice shown in Fig. 1(a). The solid line denotes data for $(4,0,0)$, solid triangles: $(3,1,0)$, open triangles: $(3,0,1)$, open squares: $(2,2,0)$, reversed triangles: $(2,1,1)$, crosses: $(1,2,1)$, and bullets: $(0,4,0)$.

with $S > 1/2$ where several sets of $\{n_M\}$ exist for a given value of M .

For boson systems ($S = 1$) we found that there is a ground state in each set of $\{n_M\}$ and that the same type of degenerate ground-state structure appears as the one found for $S = 3/2$, but in this case regardless of the value of U_0 and of the shape of the lattice, which is an intrinsic property of the bosonic case. Thus, we conclude that boson itinerant magnetic systems always have a state with the maximum total spin belonging to the manifold of ground states. This property follows quite naturally from the fact that the Hamiltonian of the boson system can be transformed such that all elements have the same sign, implying that the ground state is fully symmetrized. In contrast, for fermion systems we need an additional condition, the condition for the Nagaoka ferromagnetism, for the ground state to have maximum total spin.

We expect that these properties will be confirmed in real experimental systems.

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